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SUBJ: STATISTICAL EVALUATION OF PCB DISTRIBUTION PATTERNS
IN THE UPPER ACUSHNET RIVER ESTUARY

Introduction

Brown and Wagner (Sept., 1986) performed a detailed analysis of the PCB patterns exhibited by surficial and subsurface sediment samples taken at 24 locations in the upper part of the Acushnet River Estuary (Figure 1). For most sites, the A sample was collected at 5 - 7.5 cm, and the B sample deeper in the core at 15 - 17.5 cm. It is likely that many samples of A and all of B are anoxic if not anaerobic. The sediment samples were analyzed by high resolution glass capillary gas chromatography (HRGC) using electron capture detection. The analytical procedure yielded about 118 individual PCB congeners or sets of eluting congeners. The PCB congeners were identified, assigned an IUPAC number and given a calculated weight % (concentration) or mole %.

Based on the PCB congeneric patterns, Brown and Wagner (Sept., 1986) concluded that 1) Aroclor 1242 and 1254 PCB mixtures were the dominant mixtures released to the system; 2) PCB mixtures had undergone unquantified degrees of weathering, vertical transport and some dechlorination at sub-surface levels, but little or no aerobic microbial degradation or lateral transport between sediment sites had occurred; 3) dechlorination patterns were different from those observed elsewhere. The objective of this exercise is to apply the statistical techniques of factor and cluster analysis to determine the degree of similarity of PCB patterns site to site, and also site to site variations.

Results

The data on the PCB congeneric patterns were organized as follows. Each sample having a site designation (e.g., 2A means surface sediment at site 2) provided for about 118 peaks representing PCB congeners and corresponding to a calculated weight % concentration. An example of Brown and Wagner's data (Sample ID 2A) are given in Table 1. The entire computerized data base is given in the Appendix. Concentrations represented by peaks 2 and 3 were flagged as inaccurate

in the orginal report and were deleted from all sample compilations leaving 116 peaks. In the factor analysis, peaks 1, 40, 114, 116 and 118 of the original data sets were deleted because all concentrations were zero. This has no significant effect on the results. In the computer printouts, case or symbol corrsponds to a particular sample designation as follows:

Sample ID	Site or Case	Sample ID	Site or Case
<hr/>			
(Figure 1)			
2 A	1	18A	13
2 B	2	18B	14
5 A	3	19A	15
5 B	4	19B	16
9 A	5	21A	17
9 B	6	21B	18
12A	7	22A	19
12B	8	22B	20
14A	9	24A	21
14B	10	24B	22
17A	11	26A	23
17B	12	26B	24
		Aroclor 1242	25
		Aroclor 1254	26

Statistical analyses (factor; cluster) were performed on the data set described above using SPSS-X, a comprehensive, integrated system for managing, analyzing and displaying information. Calculations were performed on a DEC-VAX-8600 computer in the University of Minnesota Academic Computing Service and System. Data files contain the values of PCB congeneric peak number and weight % concentration of each congener measured for a set of sediment samples with identification numbers as above. The factor analysis procedure is used to identify "factors" which account for the observed correlations in PCB congener patterns at a number of sites.

Principal component analysis (Table 2) showed that > 90 % of the variability of PCB congeneric patterns at all sites could be explained by three factors. Factor 1 included all but 5 samples and consisted of PCB congeneric patterns most similar to Aroclor 1242. Factor 2 contained two samples and Aroclor 1254. Factor 3 contained only two samples. A simple varimax rotation of factor 1 and factor 2 yielded a graphical representation of the factor analysis. Cases (numbers on Figure 2 corresponding to sample ID's) heavily loaded on horizontal factor 1 were most similar to PCB congeneric distributions in Aroclor 1242. Similarly, cases heavily loaded on vertical factor 2 (numbers 13, 14) were most simialr to Aroclor 1254. Cases not heavily loaded on either (cases 10, 12) were not similar to either factor 1 or 2. Most cases were loaded similarly on factors 1 and 2 but favored horizontal factor 1.

Statistical analysis of these data is somewhat problematic in that the PCB congeneric patterns exhibited by the sediment samples are similar with a few notable exceptions. Inclusion of PCB congeneric patterns

for sediment samples in the inner and outer harbor would greatly facilitate comparisons. The factor analysis plot in Figure 2 demonstrates that 1) PCB profiles at most sites are approximated by linear combinations of Aroclor 1242 and 1254 mixtures; 2) Cases 13 and 14 in Figure 2 corresponding to samples 18A and 18B are similar to unweathered or undegraded Aroclor 1254; 3) Cases 10, 22 and to a lesser extent 24 in Figure 2 corresponding to samples 14B, 24B and 26B are dissimilar to either Aroclor 1242 and 1254. The PCB patterns in these subsurface patterns appear significantly weathered and/or degraded; 4) There is a suggestion that the most altered PCB patterns are relegated to sediment sites to the north; 5) Samples taken deeper in the core (B samples) exhibit PCB patterns more similar to Aroclor 1254 than Aroclor 1242. This could result from a combination of variable Aroclor input strengths, physical weathering or degradation. Other types of factor rotation (quartimax; equamax; oblimum) did not generate different or additional conclusions.

Cluster analysis performed on the above data set using the method of average linkage between two clusters is defined as "the average of the distances between all pairs of cases in which one member of the pair is from each of the clusters". This is the most common and usually the most preferred of several methods. A dendrogram is a physical portrayal of the clusters being combined (Figure 3). The distance (length of horizontal lines linking groups) represents the relative difference between clusters which are being combined. Long lengths mean that dissimilar clusters are being combined.

The dendrogram shows that 1) Sample 14B exhibits a PCB pattern dissimilar to all others; 2) Samples 18A, 18B, 14B and Aroclor 1254 are all dissimilar to other samples based on PCB congeneric patterns; 3) All other samples are more similar than dissimilar and gather in one large cluster. These PCB profiles then are combinations of Aroclor 1242 and Aroclor 1254 but favoring Aroclor 1242.

These statistical analyses considered with the PCB pattern interpretations of Brown and Wagner support the hypothesis that weathering and/or degradation of PCBs is occurring in the sediments of the Acushnet River estuary upstream of the inner harbor. Unfortunately, the usefulness of factor and cluster analyses to quantify this conclusion is limited by the general similarity of PCB congeneric patterns as altered by in situ reactions. That is, these samples exhibit characteristics of PCB microbial dechlorination. However, this process does not alter the whole PCB profile sufficiently to conclusively quantify this process using these procedures. The statistical procedures do, however, support the hypothesis that alterations have occurred resulting in different PCB congener profiles at different depths at the same site and at different sites.

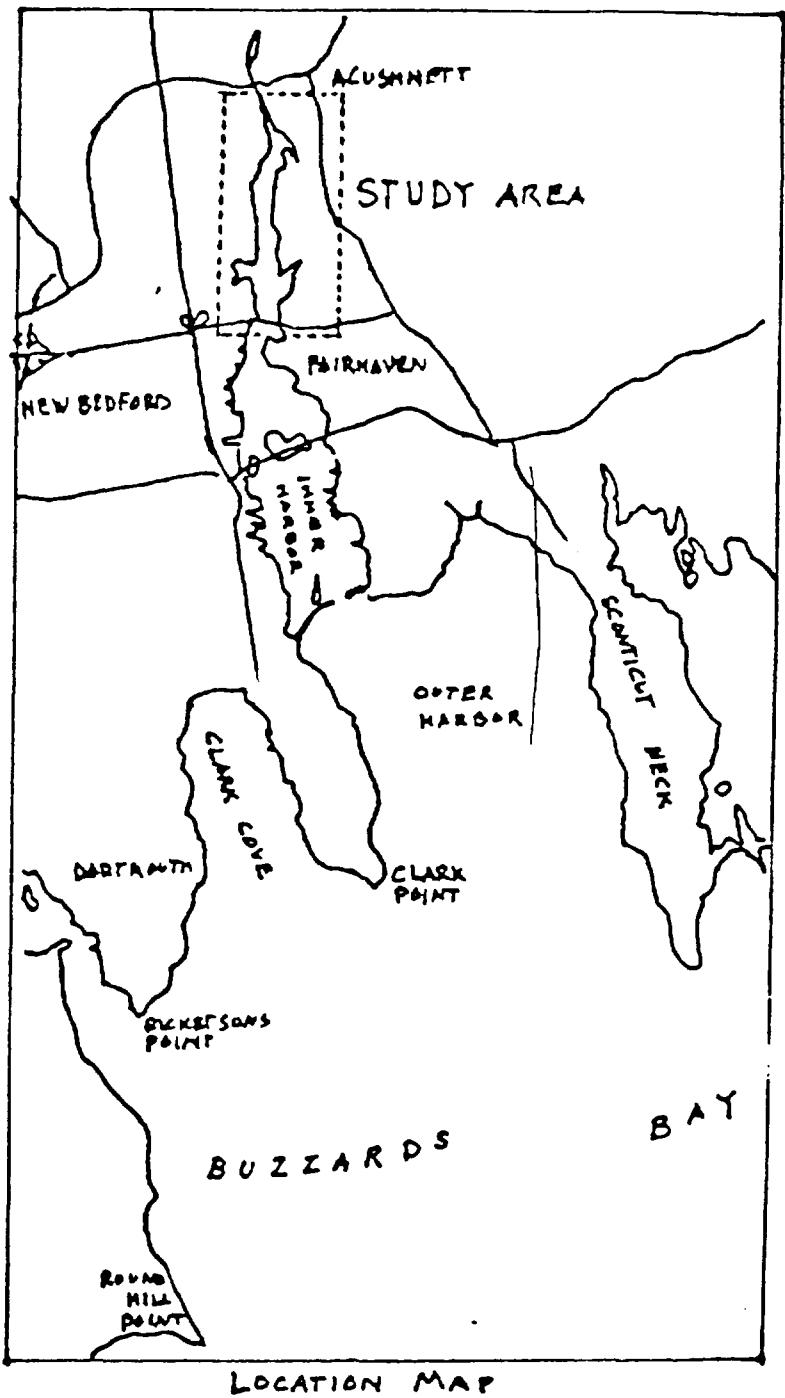
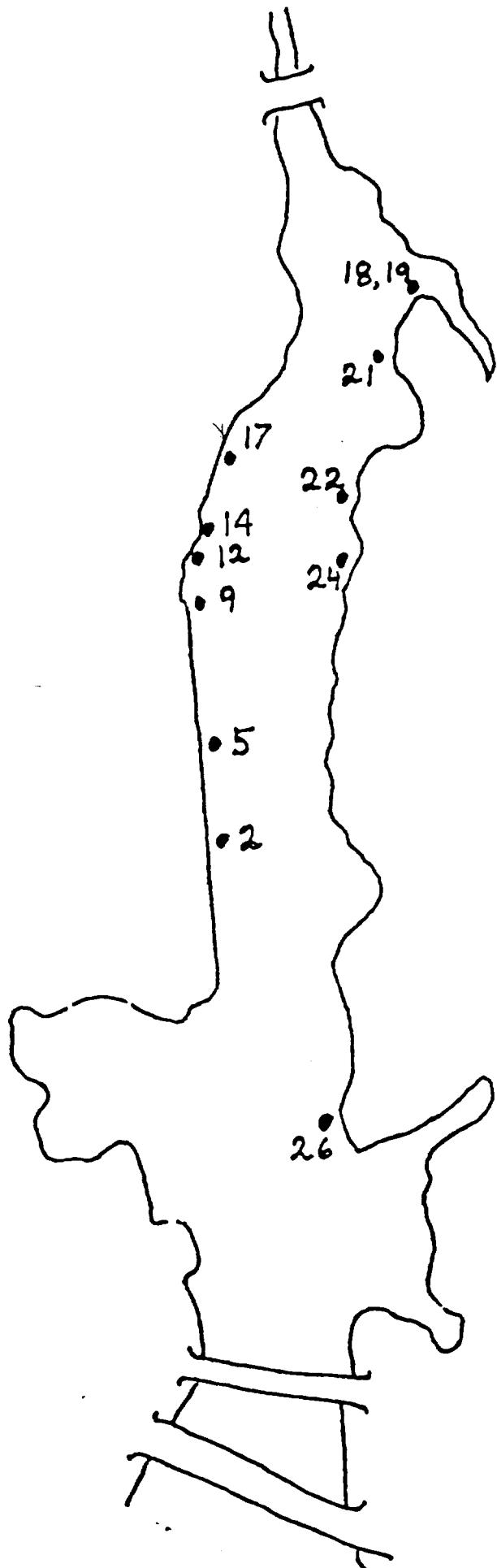


Figure 1. Map of Upper Acushnet River Estuary sediment study area, showing locations of collection sites.

N.B.

2 A Table 1A

5.	16.952 19.242 18.510 19.752 20.097 20.417 20.829 21.208 21.532	
10.	22.214 23.455 22.658 23.051	
14, 15.	23.350 23.931	
19.	23.947	
21, 22.	24.065	
23, 24.	24.974 25.818	24.974
31, 32.	26.030	25.729
37, 38.	26.530	26.771
39.	27.140	
46, 47, 48.	27.729	
49.	27.885	
53.	28.147	
58.	28.676	
61.	29.243	
68.	29.825 30.105	29.540
69.	30.640	30.345
74, 75.	30.850	31.106
82.	31.329 31.747	
87.	32.315 32.563 32.953	32.034
95.	33.145 33.664	
102.	34.072 34.390 34.701 35.006	
104.	35.375 35.660 35.974 36.344	
109.	37.141	
110.	37.483	
	38.195	
		38.700 Int. Std.
	39.174 39.432	
115.	40.778	
	41.802 42.066	
117.	44.228	

g8

2 A

3

- - - - - FACTOR ANALYSIS - - - - -

ANALYSIS NUMBER 1 LISTWISE DELETION OF CASES WITH MISSING VALUES

>WARNING 11302

>The correlation matrix is ill-conditioned.

KAISER-MEYER-OLKIN MEASURE OF SAMPLING ADEQUACY = .85776
BARTLETT TEST OF SPHERICITY = 9174.9623, SIGNIFICANCE = .00000

EXTRACTION 1 FOR ANALYSIS 1, PRINCIPAL-COMPONENTS ANALYSIS (PC)

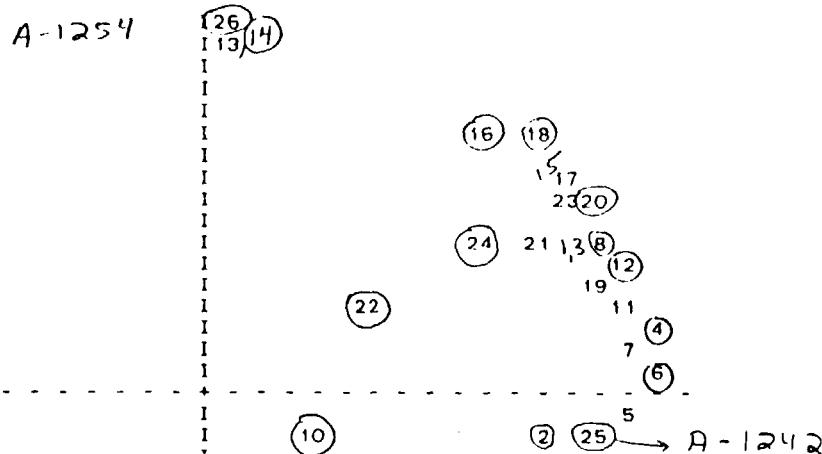
INITIAL STATISTICS:

VARIABLE	COMMUNALITY	•	FACTOR	EIGENVALUE	PCT OF VAR	CUM PCT
SITE1	1.00000	*	1	18.75529	72.1	72.1
SITE2	1.00000	*	2	3.38196	13.0	85.1
SITE3	1.00000	*	3	1.39168	5.4	90.5
SITE4	1.00000	*	4	.74588	2.9	93.4
SITE5	1.00000	*	5	.62700	2.4	95.8
SITE6	1.00000	*	6	.25342	1.0	96.8
SITE7	1.00000	*	7	.18997	.7	97.5
SITE8	1.00000	*	8	.12920	.5	98.0
SITE9	1.00000	*	9	.10798	.4	98.4
SITE10	1.00000	*	10	.10072	.4	98.8
SITE11	1.00000	*	11	.07825	.3	99.1
SITE12	1.00000	*	12	.06632	.3	99.3
SITE13	1.00000	*	13	.05948	.2	99.6
SITE14	1.00000	*	14	.04360	.2	99.7
SITE15	1.00000	*	15	.02112	.1	99.8
SITE16	1.00000	*	16	.01291	.0	99.9
SITE17	1.00000	*	17	.01122	.0	99.9
SITE18	1.00000	*	18	.00904	.0	99.9
SITE19	1.00000	*	19	.00427	.0	100.0
SITE20	1.00000	*	20	.00320	.0	100.0
SITE21	1.00000	*	21	.00238	.0	100.0
SITE22	1.00000	*	22	.00184	.0	100.0
SITE23	1.00000	*	23	.00139	.0	100.0
SITE24	1.00000	*	24	.00099	.0	100.0
SITE25	1.00000	*	25	.00046	.0	100.0
SITE26	1.00000	*	26	.00043	.0	100.0

Table 2

- - - - - F A C T O R A N A L Y S I S - - - - -

HORIZONTAL FACTOR 1 VERTICAL FACTOR 2



○ = subsurface contour

Figure 2

SYMBOL	VARIABLE	COORDINATES	SYMBOL	VARIABLE	COORDINATES	SYMBOL	VARIABLE	COORDINATES	SYMBOL	VARIABLE	COORDINATES
1	SITE1	(.84382, .39685)	2	SITE2	(.70411, -0.05631)	19	SITE19	(.82311, .26975)	20	SITE20	(.82248, .5079
3	SITE3	(.88692, .35584)	4	SITE4	(.94080, .14740)	21	SITE21	(.74535, .38461)	22	SITE22	(.36579, .2279
5	SITE5	(.91472, -0.02499)	6	SITE6	(.94705, .04043)	23	SITE23	(.80478, .51981)	24	SITE24	(.61326, .3768
7	SITE7	(.92912, .12154)	8	SITE8	(.84273, .38320)	25	SITE25	(.84731, -0.07968)	26	SITE26	(.06137, .9524
9	SITE9	(.77785, .50526)	10	SITE10	(.25114, -0.08052)						
11	SITE11	(.89367, .23336)	12	SITE12	(.91916, .30542)						
13	SITE13	(.08901, .91220)	14	SITE14	(.10489, .96395)						
15	SITE15	(.78310, .55477)	16	SITE16	(.59165, .68185)						
17	SITE17	(.80495, .54050)	18	SITE18	(.69936, .68793)						

* * * * * HIERARCHICAL CLUSTER ANALYSIS * * * * *

Dendrogram using Average Linkage (Between Groups)

Rescaled Distance Cluster Combine

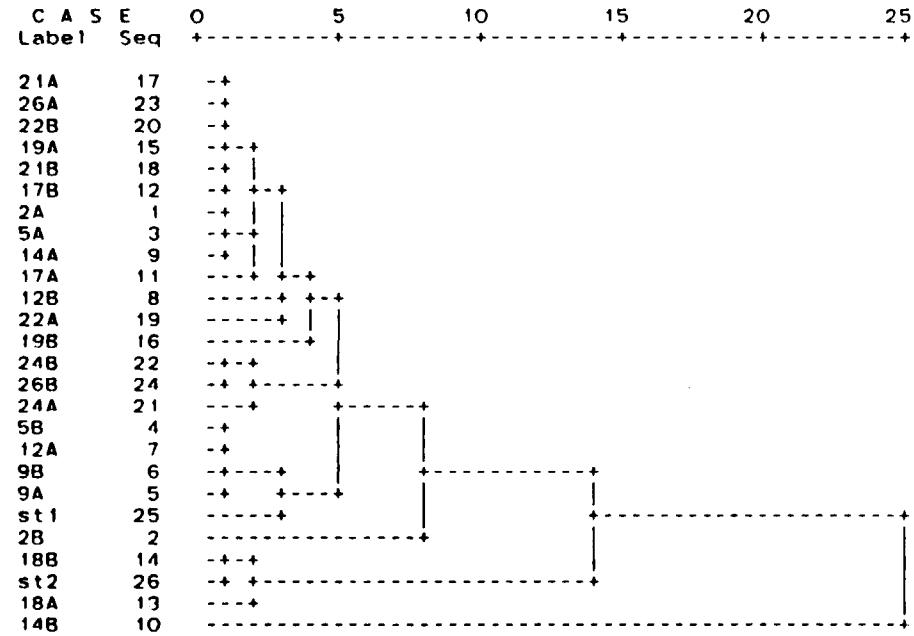


Figure 3

2A 0 0000 0 7360 0 7358 0 3549 1 4954 2 3248 0 0427
 0 4894 0 0040 0 0000 0 2401 5 6124 2 8413 0 4965 2 6799 0 0195
 0 0713 0 0512 2 5994 2 0063 5 0770 6 5779 3 0649 1 9269 0 6955
 0 0000 0 4779 0 0000 5 4206 3 5003 1 2975 0 9367 0 0000 0 1040
 3 4618 2 7200 2 7125 0 0000 0 1660 0 7657 0 2210 0 4274 0 2478
 1 4343 2 1684 2 5118 0 8065 1 8051 1 5880 0 0337 2 6448 1 6078
 0 1265 0 0000 0 8464 1 0760 0 4970 0 3067 4 0402 0 0374 0 3629
 0 3981 0 4359 0 2652 0 0000 0 0000 4 1824 0 0034 0 2866 0 1038
 0 3628 1 0375 0 0000 0 0676 0 2597 0 0000 0 2593 0 0000 0 0000
 2 2823 0 3490 0 2286 0 0577 0 0000 0 0186 0 1638 0 5177 0 0000
 0 0000 0 0196 0 1520 0 1172 0 4227 0 0000 0 0532 0 0044 0 0051
 0 0666 0 0000 0 3143 0 0013 0 0000 0 0000 0 2071 0 0537 0 0017
 0 0527 0 0515 0 0083 0 0252 0 0060 0 0000 0 0394 0 0000 0 0570
 0 0000

2B 0 0000 0 2190 2 3357 0 7154 4 6591 4 9843 0 0000
 0 9008 0 0353 0 0000 0 4848 10 6696 5 5513 1 0236 2 5019 0 0097
 0 0000 0 0229 3 9378 0 0000 7 6590 0 0000 1 5530 0 8877 0 9487
 0 0164 0 6757 0 5417 0 0000 5 2815 2 2498 0 1569 0 0000 0 1548
 3 0200 0 0000 3 6099 0 0000 0 0000 0 3751 0 1364 0 6115 0 1302
 1 5284 0 0000 3 0889 0 9351 0 9303 1 0031 1 7727 0 0000 1 3881
 0 1360 0 0088 0 5405 0 4292 0 3114 5 2638 0 0000 0 0494 0 1586
 0 2833 0 3034 0 1828 0 0000 0 0000 3 0986 0 0000 0 1929 0 0000
 0 2347 0 4431 0 0000 0 0440 0 0271 0 0000 0 1654 0 0000 0 0000
 1 1715 0 2391 0 1422 0 0286 0 0000 0 0000 0 1570 0 3098 0 0000
 0 1901 0 0194 0 1307 0 0955 0 2656 0 0317 0 0000 0 0000 0 0497
 0 0000 0 2963 0 0135 0 0000 0 0000 0 0137 0 1679 0 0000 0 0345
 0 0000 0 0000 0 0000 0 0156 0 0000 0 0000 0 0484 0 0000 0 0000
 0 0000

5A 0 0000 0 5671 1 4077 0 3285 2 1489 2 6878 0 0417
 0 6888 0 0517 0 0000 0 2461 6 2248 3 5465 0 6633 1 9631 0 0085
 0 0000 0 0201 2 4144 2 1623 4 6367 8 1435 1 7975 1 0030 0 8232
 0 0144 0 6079 0 0000 5 3435 4 2329 1 9163 1 0034 0 0000 0 1470
 2 7938 2 7572 3 1721 0 0000 0 3446 0 4715 0 1547 0 4647 0 1585
 1 6219 2 3999 3 2861 0 9294 1 3983 1 1491 0 0000 2 3760 1 7292
 0 1605 0 2698 0 7688 0 6719 0 4157 0 0000 3 2226 0 0541 0 2630
 0 3387 0 3760 0 0000 0 3144 0 0000 3 3770 0 0000 0 2359 0 0927
 0 3087 0 7080 2 7641 0 1818 0 2115 0 0925 0 2064 0 2112 0 0000
 1 6174 0 2948 0 1825 0 0418 0 0111 0 0122 0 1956 0 4307 0 0000
 0 2390 0 0227 0 1593 0 1166 0 3584 0 0457 0 0000 0 0000 0 0000
 0 0797 0 0000 0 3436 0 0000 0 0047 0 0261 0 2130 0 0566 0 0000
 0 0567 0 0721 0 0000 0 0192 0 0000 0 0000 0 0626 0 0000 0 0344
 0 0000

5B 0 0000 0 1859 1 9829 0 6073 3 9554 4 2315 0 0000
 0 7647 0 0300 0 0000 0 4116 9 0580 4 7128 0 8690 2 1240 0 0082
 0 0721 0 0194 3 3430 3 3288 6 5021 8 5169 1 3184 0 7537 0 8054
 0 0139 0 5736 0 0000 5 6045 4 4838 1 9100 0 5642 0 0000 0 1314
 2 5639 2 5607 3 0647 0 0000 0 0000 0 3184 0 1158 0 5192 0 1105
 1 2975 1 6986 2 6224 0 7938 0 7899 0 8516 0 0053 1 5999 1 1784
 0 1155 0 1866 0 4589 0 3644 0 2644 0 0000 2 2718 0 0419 0 1346
 0 2405 0 2576 0 0000 0 2126 0 0000 2 3795 0 0000 0 1638 0 0000
 0 1993 0 3761 1 9314 0 0373 0 1421 0 0704 0 1404 0 1329 0 0000
 0 9945 0 2030 0 1207 0 0243 0 0064 0 0000 0 1333 0 2630 0 0000
 0 1614 0 0165 0 1109 0 0811 0 2255 0 0269 0 0000 0 0000 0 0000
 0 0456 0 0000 0 2456 0 0079 0 0000 0 0116 0 1425 0 0000 0 0293
 0 0000 0 0000 0 0000 0 0133 0 0000 0 0000 0 0411 0 0000 0 0000
 0 0000

9A 0 0000 0 6300 3 7090 1 0615 2 6335 6 3036 0 0761

0 4580	0 0124	0 3027	0 1743	5 1473	6 1471	0 7700	1 7701	0 8878
0 0373	0 0482	1 5931	1 5064	4 3751	6 6592	2 1404	1 1944	0 6263
0 0115	0 4749	0 0000	4 8062	4 2519	1 9793	1 0056	0 0819	0 1360
2 6531	2 7540	2 9125	0 0000	0 3157	0 5073	0 1635	0 4470	0 1829
1 6810	3 6159	6 1019	1 1643	1 9073	1 2197	0 0000	3 2153	2 5586
0 2537	0 2780	0 9067	0 5315	0 2935	0 0000	3 6996	0 0738	0 1868
0 3349	0 3713	0 0000	0 3840	0 0000	4 3068	0 0000	0 2284	0 0943
0 3464	0 4995	3 2258	0 0729	0 1470	0 0742	0 1655	0 1566	0 0000
1 3445	0 2442	0 1499	0 0302	0 0089	0 0048	0 1626	0 2903	0 0000
0 2962	0 0000	0 1209	0 0847	0 2996	0 0000	0 0247	0 0000	0 0000
0 0523	0 0000	0 2413	0 0079	0 0037	0 0145	0 1585	0 0476	0 0000
0 0383	0 0478	0 0000	0 0000	0 0000	0 0000	0 0376	0 0000	0 0000
0 0000								

14B	0 0000	0 0000	0 8087	0 0629	0 4494	0 3936	0 3223	
	0 0708	0 1740	0 0000	0 0000	25 1030	0 7302	0 7725	0 0000 9 2142
	0 0000	10 2381	0 5286	2 1046	1 2209	1 2214	0 9327	0 1578 0 1769
	0 0000	0 9850	0 0000	1 2528	1 0753	0 4567	0 2045	0 0717 0 0000
	0 5305	0 6506	0 5489	0 0000	0 1659	0 1176	0 0000	0 0000 0 0401
	0 3268	0 5982	0 9011	0 2311	0 4193	0 2727	0 0000	0 5411 0 3710
	0 0290	0 0325	0 1506	0 1384	0 1111	0 0000	0 6131	0 0000 0 0475
	0 0595	0 0000	0 0000	0 0631	0 0000	0 6635	0 0000	0 0281 0 0000
	0 0433	0 1321	0 5343	0 0813	0 0318	0 0000	0 0000	0 0000 0 0000
	0 2580	0 0345	0 0000	0 0000	0 0000	0 0000	0 0381	0 0515 0 0000
	0 0000	0 0000	0 0000	0 0000	0 0323	0 0000	0 0000	0 0000 0 0000
	0 0000	0 0000	0 0000	0 0000	0 0000	0 0000	0 0139	0 0000 0 0000
	0 0000	0 0000	0 0000	0 0000	0 0000	0 0000	0 0000	0 0000 0 0000
	0 0000							

17A	0 0000	0 1759	1 1720	0 6290	2 3448	3 1987	0 0637	
	0 6462	0 0378	0 2593	0 5122	6 4245	3 6265	0 6289	3 0737 0 0078
	0 1023	0 0551	2 7515	2 2603	5 3080	7 8260	2 8567	2 1839 0 8463
	0 0263	0 6281	0 0336	4 4960	3 9415	1 8447	0 9782	0 0663 0 1554
	3 3955	3 1116	0 0277	0 0000	2 8853	0 8068	0 1803	0 5892 0 2554
	1 4639	2 1928	4 3872	0 9399	1 9387	1 0820	0 0000	2 0530 1 7302
	0 1806	0 2753	0 7369	0 2434	0 1222	0 0000	2 4760	0 0595 0 0860
	0 2481	0 2310	0 0000	0 2925	0 0000	2 3465	0 0000	0 1671 0 0620
	0 2403	0 2001	1 8745	0 1237	0 0751	0 0666	0 0925	0 0000 0 0000
	0 7104	0 1470	0 0774	0 0268	0 0000	0 0000	0 1161	0 1524 0 0000
	0 1460	0 0104	0 0588	0 0367	0 1515	0 0182	0 0035	0 0000 0 0000
	0 0000	0 1401	0 0000	0 0000	0 0029	0 0184	0 0805	0 0296 0 0178
	0 0000	0 0364	0 0042	0 0050	0 0018	0 0016	0 0266	0 0000 0 0472
	0 0000							

17B	0 0000	0 1609	1 1259	0 4254	3 1287	2 9266	0 0816	
	0 7039	0 0000	0 3164	0 5436	6 1888	3 4074	0 5623	2 4853 0 0071
	0 0000	0 0056	4 6769	3 9424	6 0788	6 8832	1 7056	1 6494 0 6757
	0 0000	0 5094	0 0000	6 2890	5 1212	2 2035	0 5560	0 0856 0 0663
	3 0281	2 5881	2 4017	0 0000	0 3465	0 5302	0 3064	0 8325 0 1859
	0 7878	0 9331	1 3157	1 4981	0 7852	1 4601	0 0000	2 2893 2 5669
	0 3650	0 3100	0 8502	0 1627	0 0494	0 3641	3 4789	0 1225 0 0252
	0 3973	0 2882	0 0000	0 3805	0 0000	2 7698	0 0000	0 1865 0 0687
	0 3492	0 0000	3 1224	0 1178	0 0325	0 0997	0 0920	0 0000 0 0000
	0 7395	0 1345	0 0336	0 0385	0 0000	0 0000	0 1943	0 0574 0 0000
	0 1821	0 0095	0 0445	0 0305	0 1104	0 0133	0 0000	0 0000 0 0000
	0 0364	0 1444	0 0139	0 0000	0 0000	0 0000	0 0736	0 0339 0 0235
	0 0000	0 0521	0 0000	0 0000	0 0000	0 0000	0 0337	0 0000 0 0000
	0 0000							

18A	0 0000	0 8119	0 0000	0 0421	0 0215	0 1013	0 7059	
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1 4512	0 0228	0 4452	0 0000	0 5001	0 2819	0 3630	0 2801	0 0120
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